

# Python in Fluidity

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August 15, 2008

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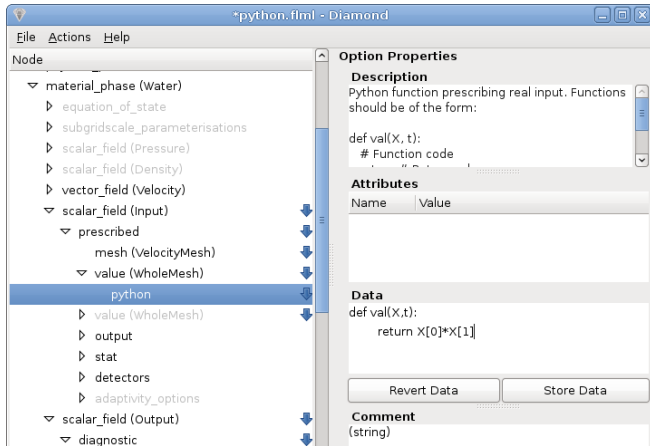
- Passing Arrays to Python
- `shape_dshape()`

# Goals of This UROP

- Make Fluidity more accessible towards users' requirements by having a Python environment available
- Pass data structures from Fortran to Python in a memory efficient way
- Give some functionality of the Fortran code in the Python environment

# Previous Functionality

- `set_from_python()`
- Passed tuple to return the values for each node in the field



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# Setup and Basics for the Python Environment

## Initialization and Finalization in *main.cpp*

- `#include "python_statec.h"` as external
- `python_init_()` (note the underscore!)
- `python_end_()`
- Call only once before and after the main program.
- `export PYTHONPATH=fluidityroot/python/`

## Cleaning Up and Resetting

- `python_reset_()`
- Clears all python dictionaries apart from the essential ones (`__doc__`, `numpy`, `string`, etc.)
- Exception: *persistent*{ } - use this dictionary to keep data from being deleted

# Running Python Code in Fluidity

## In Fortran

- `python_run_string(string code)`, e.g. `"a = 5; print a"`
- `python_run_file(string filename)` - Better to write a module and import via `run_string()` though
- `python_add_state(state_type State)`

## In Python

- Last added state always available as `state`
- All added states: `states{'State1','MyState','Water'}`
- Load modules from the `./python` folder, e.g. `import fluidity.ocean_biology`
- A state has different attributes:
- `scalar_fields`, `vector_fields`, `tensor_fields` (passed by reference)





# Set Diagnostic Fields From Python

## Diamond Functionality

- Scalar field to be set available as *field*
- All states available in *states*

The screenshot shows the Diamond GUI window titled '\*python.flml - Diamond'. The left pane displays a tree of nodes under 'material\_phase (Water)'. The 'diagnostic\_algorithm' node is selected. The right pane shows the 'Option Properties' for this node, including a description, attributes table, data code, and a comment.

**Node**

- material\_phase (Water)
  - equation\_of\_state
  - subgridscale\_parameterisations
  - scalar\_field (Pressure)
  - scalar\_field (Density)
  - vector\_field (Velocity)
  - scalar\_field (Input)
  - scalar\_field (Output)
    - diagnostic
      - mesh (VelocityMesh)
      - diagnostic\_algorithm
    - output
    - stat
    - detectors
    - adaptivity\_options
  - scalar\_field
  - vector\_field

**Option Properties**

**Description**

Algorithm for the diagnostic value coded in Python. The object 'state' has the attributes 'scalar\_fields', 'vector\_fields' and 'tensor\_fields'; 'field' is the diagnostic field to be set

**Attributes**

Name	Value
------	-------

**Data**

```
cf = state.vector_fields['Coordinate']  
for i in range(field.val.shape[0]):  
    field.val[i] = cf.val2[i] * cf.val1[i]
```

**Comment**

Python in Fluidity

# Noteworthy Functions From Fortran Available in the Python Interpreter

## Field Methods

- `ele_val(int ele_number)` - Return the values of field at the nodes of `ele_number`
- `ele_val_at_quad(int ele_number)` - Return the values of field at the quadrature points of `ele_number`

## Mesh Methods

- `ele_nodes(int ele_number)` - Return all nodes associated with the element `ele_number`

## Transform Methods

- `transform_to_physical_detwei(Field field)`
- `grad(int gi, Element shape)`
- `shape_shape(Element shape1, Element shape2)`

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# Affected Files

## Fortran

- /femtools/python\_state.F90
- /assemble/Diagnostics\_fields\_wrapper.F90

## C/C++

- /main.cpp
- /include/python\_statec.h
- /femtools/python\_statec.c

## Python

- /python/fluidity/state\_types.py

## Set a Diagnostic Field From Python

```
subroutine set_diagnostic_field_from_python(state,field)
  type(state_type),intent(inout) :: state
  type(scalar_field), intent(inout) :: field
  character(len=PYTHON_FUNC_LEN) :: pycode
#ifdef HAVE_NUMPY
  ! Clean up to make sure that nothing else interferes
  call python_reset()
  call python_add_state(state)
  call python_run_string(" field =
state.scalar_fields['" // trim(field%name) // "' ]")
  call
  get_option(trim(field%option_path) // "/diagnostic/diagnostic_algorithm",pycode)
  call python_run_string(trim(pycode))
#else
  FLAbort("Python diagnostic fields require NumPy, which cannot be
located.")
#endif
end subroutine set_diagnostic_field_from_python
```

# Passing one of the fields (Fortran)

```
python_add_scalar()
```

```
interface
  subroutine
    python_add_scalar(sx,x,name,nlen,field_type,option_path,oplen,state_name,snlen,&
      &mesh_name,mesh_name_len)
    integer :: sx,nlen,field_type,oplen,snlen,mesh_name_len
    real, dimension(sx) :: x
    character(len=nlen) :: name
    character(len=snlen) :: state_name
    character(len=oplen) :: option_path
    character(len=mesh_name_len) :: mesh_name
  end subroutine python_add_scalar
end interface
```

# Passing one of the fields (C)

```
python_add_scalar_()
```

```
void python_add_scalar_(int *sx, double x[],char *name,int *nlen,  
int *field_type, char *option_path,int *oplen, char *state_name,int *slen,  
char *mesh_name, int *mesh_name_len)
```

- Note the `_`, appended to every function name from Fortran in C
- All values passed by reference (pointers!)
- Fortran strings are not null-terminated (call `char* fix_string(char *s, int len)` and free value after use)



# Setting Up Data For Python

## Setting Strings

- Null-terminate strings with char *\*namec = fix\_string(name, \*nlen)*
- PyObject *\*pname = PyString\_FromString(namec);*
- PyObject *\*pMain = PyImport\_AddModule("\_\_main\_\_");*
- PyObject *\*pDict = PyModule\_GetDict(pMain);*
- *PyDict\_SetItemString(pDict, "n", pname);*
- *Py\_DECREF(pname)* when cleaning up to allow garbage collection by Python interpreter

## Setting integers/reals/doubles and objects

- char *c[60];* // Allocate a string large enough for the command
- *sprintf(c, "pynumber = %d", \*myint);*
- *PyRun\_SimpleString(c);* //Execute the command

## (C) Passing It All In

### Creating a NumPy Array (see also Final Notes)

- `int dims[] = {*size};`
- `PyObject *arr = PyArray_FromDimsAndData(  
    • 1, - dimensions  
    • dims, - size in each dimension  
    • PyArray_DOUBLE, - data type, alt. PyArray_INT  
    • (char*)data); - pointer to the array`
- `PyDict_SetItemString(pDict," myPyArray",arr);`

### (C) Creating the Object in Python

- `char c[150+*slen+*mesh_name.len];`
- `// Create command with the variables we set  
printf(c," field = ScalarField(n,myPyArray,ft,op);  
states['%s'].scalar_fields['%s'] = field", n, namec);`
- `PyRun_SimpleString(c); //Execute the command`

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# Passing Arrays to Python

(F) `python_add_array(real* myArray, string arrayName)`

- Valid for 1-, 2- and 3-dimensional integer and real arrays
- E.g.: `real, dimension(:, :, :) :: myFortArray`
- `python_add_array(myFortArray, "thisIsMyNameInPython")`

(C) `python_add_array_double_2d(double* myArray, int *sx, int *sy, char* arrayName)`

- Fortran wrapper functions as well as C standalone functions available in `python_statec.c`
- Functions for integers and doubles, 1d, 2d, 3d

# `shape_dshape()`

## (Py) `Transform.shape_dshape()`

- Equivalent to Fortran `shape_dshape()`
- Create Transform object to calculate Jacobian and Detwei
- Calculate dshape with `Transform.grad(coordinateField)`
- Call `shape_dshape(shape,dshape)`
- Example in `state_types.py`